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**Final Report**

1. Grant Title: "Computational Studies of Strongly Interacting Electrons"
2. Principal Investigator: Prof. Elbio Dagotto (Florida State University). Co-PI's: Prof. Adriana Moreo (Florida State University) and Prof. Richard T. Scalettar (Univ. of California at Davis).
3. Grant Number: ONR-N00014-94-1-1031 (ASSERT supplement to ONR-N00014-93-1-0495)
4. Funding Profile: the total grant amount was \$172,020. Grant period: 08/08/94 to 08/30/97.
5. Technical Objectives:
  - Study the phase diagram of models of strongly correlated electrons for the high temperature superconductors.
  - Study the development of magnetism as a function of band filling, temperature, and ratio of correlation energy to bandwidth, in tight binding models.
  - Compare theoretical predictions for angle-resolved photoemission with existing experimental data.
6. Published papers resulting from this support:
  - a. Submitted but not published: 02
  - b. Published in refereed journals: 05
  - c. Published in non-refereed journals: 01
7. Number of technical reports submitted: 0
8. Number of books written: 0
9. Number of book chapters written: 0      DTIC QUALITY INSPECTED 3
10. Patents as a result of this work.

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a. Number of applications filed: 0  
b. Number of patents granted: 0

11. Total number of presentations given: 15

- Daniel Duffy: "Specific Heat of the 2D Hubbard Model", 1997 March Meeting of the American Physical Society, Kansas City, Missouri, March 1997. The specific heat of the 2D Hubbard model was calculated using Quantum Monte Carlo techniques.
- Carey Huscroft: "Dynamical Quantities of the Disordered, Attractive 2D Hubbard Model via Quantum Monte Carlo Simulations", 1997 March Meeting of the American Physical Society, Kansas City, Missouri, March 1997. For the first time using Quantum Monte Carlo techniques various dynamical quantities related to disorder-driven phase transitions are calculated.

12. Honors and awards received during the granting period:

- C. Huscroft: Associated Western University Fellowship, for research to combine electronic calculation techniques with Quantum Monte Carlo methods and study materials in which strongly-correlated electrons play a significant role. 1996-1997. (Dr. C. Huscroft is a graduate student supported by the present ONR grant at U.C. Davis).
- D. Duffy: Finalist Fischer Graduate Florida State University for research on "Theories for High-T<sub>c</sub> Superconductors", April 1996. (Dr. D. Duffy was a graduate student supported by the present ONR grant at Florida State University. He received his PhD degree in July 1997).

13. Number of different post-docs supported at least 25% of the time for at least one calendar year: 0. Total person-months of post-doc supported under this grant: 0.

14. Number of different graduate students supported at least 25% of the time for at least one calendar year: 4. Total person-months of graduate student support under this grant: 60.

15. Most significant publications resulting from this work:

- "Influence of Next-Nearest-Neighbor Electron Hopping in the Static and Dynamical Properties of the 2D Hubbard Model ", D. Duffy and A. Moreo, Phys. Rev. B **52**, 15607 (1995). In this paper the influence of electron hopping at distance larger than one lattice spacing is analyzed. This hopping is shown to be needed to properly fit experimental photoemission data with theoretical models.
- "Effect of Disorder on Charge Density Wave and Superconducting Order in the Half-Filled Attractive Hubbard Model", C. Huscroft and R. T. Scalettar, Phys. Rev. B **55**, 1185 (1997). This paper studies the influence of on-site disorder on the phase diagram of the attractive Hubbard model at the particular density of half-filling.
- "Hole Doping Evolution of the Quasiparticle Band in Models of Strongly Correlated Electrons for the High-T<sub>c</sub> Cuprates", D. Duffy, A. Nazarenko, S. Haas, A. Moreo, J.

Riera, and E. Dagotto, accepted in Phys. Rev. B. The evolution of the quasiparticle band in the  $U - t - t'$  model for cuprates is studied using a variety of techniques. Good agreement with photoemission experiments for the cuprates is found.

- "Perpendicular Order in Frustrated Magnetic Layers", M. Enjalran, S.M. Kauzlarich, and R.T. Scalettar, to appear in "Computer Simulation Studies in Condensed Matter Physics—Recent Developments," Springer Proceedings in Physics, D.P. Landau and H.-B. Schuttler (eds), Springer-Verlag.

16. Major accomplishments:

- The influence of electron hopping at distances larger than one lattice spacing was determined. This term is crucial to properly reproduce photoemission experimental results for the high-T<sub>c</sub> superconductors.
- The nature of the superconducting-insulator phase transition in 2D disordered superconductors was determined.
- The specific heat of the 2D Hubbard model was calculated using Quantum Monte Carlo methods, allowing a comparison with experimental data for the cuprates.
- New techniques to simulate interacting electron systems were developed, including Quantum Monte Carlo, Strong Coupling Expansions, and Conserving Approximations.
- The evolution of the quasiparticle band in the 2D Hubbard and t-J models was calculated using numerical techniques. Results are in good agreement with angle-resolved-photoemission data for the cuprates.
- Phase diagrams of magnetism, e.g. in 2-D Layered Materials, were determined using Classical and Quantum Monte Carlo methods.

17. Transitions: None

18. Summary of the overall impact of the research:

Quantum simulation techniques were applied to a number of the most outstanding problems in the physics of solids, with a particular emphasis on magnetism and superconductivity. In addition, these techniques were further developed in significant new directions. Several experimental results have been explained by our theoretical calculations and simulations, specially in the area of angle-resolved photoemission experiments. New theories for the high-temperature superconductors have been analyzed with numerical techniques. Metamagnetic transitions and ferromagnetism have been studied in the context of strongly correlated electrons.

The original objectives of the proposal have been accomplished. A vast amount of additional information on models of correlated electrons has been documented. New directions of research have been identified.

19. Key words describing the project:

High-T<sub>c</sub> Superconductors, Quantum Simulations, Magnetism, D-wave Pairing.

20. Viewgraphs: one set enclosed.